

DEVELOPMENT OF WAYS TO INCREASE EFFICIENCY OF ISOPRENE PRODUCTION BY "DIOXANE" METHOD IN PRESENCE OF ZEOLITES OF GROUP OF $\text{Ca}_x[\text{H}_2\text{O}]_y\text{Al}_a\text{Si}_b\text{O}_c$

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By the methods of quantum chemistry and molecular dynamics, the possibility of increasing the selectivity of the formation of the 4,4-dimethyl-1,3-dioxane by the Prins reaction, which is a key intermediate in the synthesis of isoprene by the "dioxane" method, has been studied.

We have considered the stabilization of the transition state (TS) of this reaction on zeolites $\text{Ca}_x[\text{H}_2\text{O}]_y\text{Al}_a\text{Si}_b\text{O}_c$ with pores of different sizes (Table, Fig.). It is shown that the stabilization of the TS of the reaction for the formation of 1,3-dioxane becomes most advantageous on the zeolites of the considered group with pore sizes of 6.04–7.37 Å. Obviously, in this case the TS can be placed inside the pore of the zeolite and stabilized by intermolecular interactions with the entire inner surface of the pore.

With a pore diameter of less than 6.04 Å, the TS is no longer able to fit inside and only partially stabilizes due to interaction with the zeolite surface. In the case of zeolites with a large pore diameter, intermolecular interactions can be carried out with a fragment of the inner or outer surface of the pore.

Table. The dependence of the adsorption energy of transition states on the pore diameter of zeolites, kJ/mol

Zeolite	d, Å	ethylene	propylene	buthene-1	isobuthylene	trance-2-buthene
PAR	4,21	12.3	15.4	17.2	16	16.9
GIS	4,97	12.9	14	14.7	15.5	15.3
EPI	5,47	20.9	22.8	25.6	20.3	22
LAU	6,04	33	36.1	27.7	26.1	26.4
LEV	7,1	29.3	34.5	38.5	38.5	35.7
CHA	7,37	26.2	30.7	33.8	34.4	34.4

This type of TS stabilization indicates the possibility of increasing the selectivity of the formation of 1,3-dioxanes by the Prins reaction in the presence of zeolites of the considered group with pore sizes from 6.04 to 7.37 Å. In the case of zeolites $\text{Ca}_x[\text{H}_2\text{O}]_y\text{Al}_a\text{Si}_b\text{O}_c$, as the reacting alkene increases (from C2 to C4 chain), the diameter also increases from 6.04 Å (ethylene and propylene) to 7.1 Å (alkenes C4).

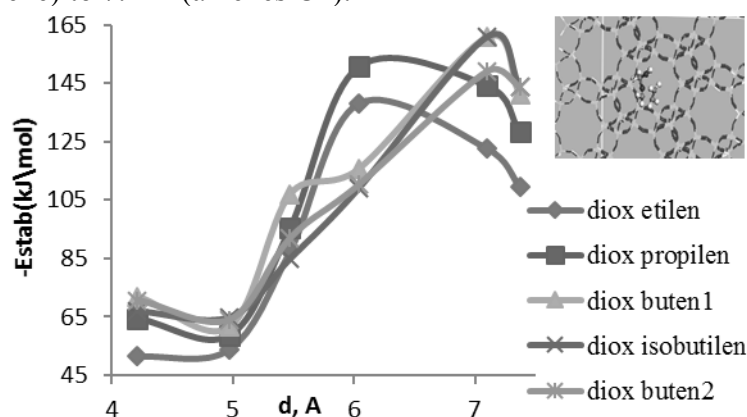


Fig. Stabilization of the transition state of the reaction of the formation of 1,3-dioxanes in the presence of group zeolites $\text{Ca}_x[\text{H}_2\text{O}]_y\text{Al}_a\text{Si}_b\text{O}_c$

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